

Amendment to the Specification

Please delete the paragraph starting on page 10, line 7 of the specification immediately following the heading "Topomer Similarity" and continuing through the equation on page 10, line 19. Please substitute the following:

The notion of topomer similarity between a pair of molecules is defined as the "distance" represented by the difference between the molecular fields which serve to characterize the molecules' shapes. As an example, assume two molecules A and B which have each been placed in their topomeric alignment and the steric field values calculated for each point in the surrounding three dimensional grids. Let each grid point be denoted by its corresponding cartesian x,y,z coordinate so for each molecule the grid points are defined as:

$$(x_0, y_0, z_0) + \dots (x_n, y_n, z_n)$$

For each molecule A and B the field values, V^A and V^B , at each point in the grid are denoted as:

$$V^A_{x_0, y_0, z_0} \dots V^A_{x_n, y_n, z_n}$$

and

$$V^B_{x_0, y_0, z_0} \dots V^B_{x_n, y_n, z_n}$$

The root sum square of distances between the field is then defined as:

$$\sqrt{(V^A_{x_0, y_0, z_0} - V^B_{x_0, y_0, z_0})^2 + \dots (V^A_{x_n, y_n, z_n} - V^B_{x_n, y_n, z_n})^2}$$

This distance is conveniently denoted as:

$$\sqrt{(A : B)^2}$$